Numeric Reasoning with Relative Orders of Magnitude

Philippe Dague

L.I.P.N. Université Paris Nord Avenue Jean-Baptiste Clément 93430 Villetaneuse - France e-mail: dague@lipn.univ-paris13.fr

Abstract

In [Dague, 1993], a formal system ROM(K)involving four relations has been defined to reason with relative orders of magnitude. In this paper, problems of introducing quantitative information and of ensuring validity of the results in \mathbb{R} are tackled.

Correspondent overlapping relations are defined in \mathbb{R} and all rules of ROM(K) are transposed to \mathbb{R} . The obtained system ROM(\mathbb{R}) depends on two independent numbers which may be freely chosen for each application. Unlike other proposed systems, a sound calculus is thus ensured in \mathbb{R} , while keeping the ability to provide commonsense explanations of the results.

These results can be refined by using additional techniques. In this way, k-bound-consistency, which generalizes interval propagation, is evaluated. Using computer algebra to push symbolic computation as far as possible and delay numeric evaluation considerably improves the results. Exact results may even be obtained by computing the roots of partial derivatives and then the extrema of symbolic expressions. It is also sometimes possible to transform rational functions so that each variable occurs only once: interval propagation then gives the exact results.

 $ROM(\mathbb{R})$, possibly supplemented by these various techniques, constitutes a rich, powerful and flexible tool for performing mixed qualitative and numeric reasoning, essential for engineering tasks.

Introduction

The use of qualitative reasoning has expanded considerably these last years, the principal field of application being the behavioral modeling of complex physical systems, in view of design, diagnosis or supervision, when purely numeric models are too complex or when available knowledge is imprecise or uncertain. For these intelligent engineering tasks, qualitative reasoning methods are required that are sufficiently flexible and subtle to be able to incorporate numeric processing and be implemented efficiently. Most of the existing approaches [de Kleer Brown, 1984, Forbus, 1984, Bobrow, and 1985, Kuipers, 1986, Dormoy and Raiman. 1988, Murthy, 1988, Struss, 1988, Williams, 1988, Travé-Massuyès and Piera, 1989] do not fulfil these requirements satisfactorily.

We are concerned here with the relative orders of magnitude paradigm, which is rich enough to capture a type of commonsense reasoning used by experts ("close to", "negligible w.r.t."), when simplifying problems or qualitatively expressing variations of a parameter between different functioning modes, and more precisely concerned with orders of magnitude expressed by binary relations r invariant by homothety (A r B depends only on A/B).

The first attempt to formalize such reasoning appeared with the formal system FOG [Raiman, 1986] (see also [Raiman, 1991] for a more general set-based framework), based on 3 basic relations and described by 32 inference rules, which has been used successfully in the DEDALE system of analog circuit diagnosis [Dague et al., 1987] for reasoning about the current intensities, which are not directly observable. Nevertheless, FOG has several limitations which prevent it from being really used in engineering. A first difficulty arises when wanting to express a gradual change from one order of magnitude to another: only a steep change is possible, due to the non overlapping of the orders of magnitude. This can be solved, as described in [Dague, 1993], by introducing a fourth relation "to be distant from" which allows overlapping relations to be defined and used. This has given a formal system ROM(K) with 15 axioms, consistency of which was proved by finding models in non standard analysis.

But two crucial problems remain: the difficulty to incorporate quantitative information when available (in DEDALE this lack of a numeric-symbolic interface meant writing Ohm's law in an ad hoc form) and the difficulty to control the inference process, in order to obtain valid results in the real world. These problems were pointed out in [Mavrovouniotis and Stephanopoulos, 1987] but the proposed system O(M) does not really solve them. In particular, use of heuristic interpretation semantics just ensures the validity of the inference in \mathbb{R} for one step (application of one rule) but not for several steps (when chaining rules). This second paper focuses on solving these two problems by concentrating on how to transpose the formal system ROM(K) to \mathbb{R} with a guarantee of soundness and how, using techniques of interval calculus and computer algebra, to build a powerful tool qualitative/symbolic for both and quantitative/numeric calculus for engineering purposes.

The present paper is organized as follows. Section 2 recalls the main features of ROM(K). Section 3 shows through an example how ROM(K), as FOG or O(M), may lead to results that are not valid in \mathbb{R} . In section 4 a translation in R of axioms and properties of ROM(K) is given, which ensures soundness of inference in \mathbb{R} . In section 5 the example is revisited with this new formulation; this time correct results are obtained. Nevertheless they may be far from the optimal ones and too inaccurate for certain purposes. In section 6 numeric and symbolic algebra techniques are proposed to refine these results: applications of consistency techniques for numeric CSPs; use of computer algebra to push symbolic computation as far as possible and delay numeric evaluation, which considerably improves the results; symbolic calculus of derivatives and of their roots by using computer algebra alone in order to compute extrema and obtain optimal results; formal transformation of rational functions by changing variables, which allows the exact results to be obtained, in particular cases, by a simple numeric evaluation and opens up future ways of research.

The Formal System ROM(K)

See [Dague, 1993] for a complete description. Quantities are taken in a totally ordered commutative field K. [A] stands for the sign of A induced by the total order \leq of K and |A| for the absolute value of A. The logical implication, equivalence, and, or, not, are written as: " \mapsto ", " \leftrightarrow ", ",", "or", " \neg " respectively (considering axioms and properties as rewriting rules of a symbolic deduction system ROM). The formal system ROM(K) involves four binary relations \approx , \sim , \ll and \neq , intuitive meanings of which are "close to", "comparable to", "negligible w.r.t." and "distant from" respectively. The 15 axioms are as follows:

(AI)	$A \approx A$
(A2)	$A \approx B \mapsto B \approx A$
(A3)	$A \approx B, B \approx C \mapsto A \approx C$
(A4)	$A \sim B \mapsto B \sim A$
(A5)	$A \sim B, B \sim C \mapsto A \sim C$
(A6)	$A \approx B \mapsto A \sim B$
(A7)	$A \approx B \mapsto C.A \approx C.B$
(A8)	$A \sim B \mapsto C.A \sim C.B$
(A9)	$A \sim 1 \mapsto [A] = +$
(A10)	$A \ll B \iff B \approx (B+A)$
(A11)	$A \ll B, B \sim C \mapsto A \ll C$
(A12)	$A \approx B$, $[C] = [A] \mapsto (A+C) \approx (B+C)$
(A13)	$A \sim B$, $[C] = [A] \mapsto (A+C) \sim (B+C)$
(A14)	$A \sim (A + A)$
(A15)	$A \neq B \iff (A-B) \sim A \text{ or } (B-A) \sim B$

Two axioms are in fact definitions: (A10) defines ≪ in terms of \approx (a quantity is negligible w.r.t. another iff the quantity obtained by adding it to the second one remains close to this second one) and (A15) defines \neq in terms of ~. (two quantities are distant iff their difference is comparable to one of them). Thus, there are only two basic relations \approx and \sim , the properties of which are given by the other 13 axioms. These basic relations are not independent but coupled by the axioms (A6) (~ is coarser than \approx) and (A11) (if two quantities are comparable, any quantity which is negligible w.r.t. the first one is also negligible w.r.t. the second one) which, using (A10), can be rewritten as: (A11') $B \sim C$, $B \approx (B+A) \mapsto C \approx (C+A)$ (if two quantities are comparable and if adding a third quantity to the first one gives a close quantity, then adding the same quantity to the second one will also give a close quantity). From (A1) to (A6) it results that both \approx and \sim are equivalence relations. (A7) and (A8) state that both \approx and \sim are stable by homothety and thus entirely determined by the class of 1 for \approx and the class of 1 for \sim . (A9) introduces a coupling between these relations and signs: a consequence is that two elements which are comparable have the same sign. (A12) and (A13) state that both relations \approx and \sim between two quantities are preserved by adding a quantity of the same sign, i.e. when moving the two quantities away from 0 by the same amount. By using invariance by homothety this is equivalent to saying that if two quantities are close (resp. comparable) then any quantity between them (for the order of K) is close (resp. comparable) to them. Finally, (A14) states that, by adding a quantity to itself, one obtains a comparable quantity (by using other axioms, it is simply equivalent to say that there exist at least two different standard positive rational numbers that can be compared by the relation (A ~ B or A \leq B)).

In [Dague, 1993], 45 properties of ROM(K) have been deduced from the previous axioms; they all have a clear intuitive qualitative meaning and illustrate the qualitative dependencies between the four relations. In particular it is proved that \ll and \neq are also stable by homothety. « is proved to be a strict order between equivalence classes for \sim (other than the class reduced to 0), and \neq a symmetric relation between equivalence classes for \approx . The relationship between \neq and \approx is clarified by the following result: if two quantities are close, then any quantity which is distant from one is distant from the other and the two distances are close. A completeness result of this qualitative representation is obtained: any given two elements are always related by \sim or (not exclusively) bv ⊈.

In addition to the introduction of the new relation \neq and the numerous associated properties, the main difference between ROM(K) and FOG or O(M) is that it is not assumed, as in FOG and O(M), that (A ~ B or A \leq B) is a total preorder on positive elements, i.e. that ~ is nothing else than the negation of \leq on positive elements:

 $A \sim B \iff \neg(A \ll B) \land \neg(B \ll A) \land [A] = [B]$. for non zero A,B, or, equivalently, that \neq is nothing else that the negation of \approx on non zero elements: $A \neq B \iff \neg(A \approx B)$ for non zero A,B.

In fact, a series of models of ROM(K) depending on one parameter is found in the field K = R of real numbers of non standard analysis, such that the above property of FOG and O(M) is not satisfied in these models. Not only does this prove the consistency of the axioms of ROM(K), but it also allows overlapping relations to be defined, that smoothly express the changes in order of magnitude, which was impossible with FOG or O(M). Instead of the 3 non overlapping relations \approx , $\neg \approx \land \sim$, \ll between two positive quantities A < B, the result is 7 basic relations that now overlap:

 $A \approx B, \neg (A \neq B), \neg (A \approx B) \land A \sim B, A \neq B \land A \sim B, A \neq B \land A \sim B, A \neq B \land \neg (A \ll B), \neg (A \sim B), A \ll B.$

Taking into account signs and identity, these 7 basic relations give 15 primitive overlapping relations between quantities of the same sign, to be compared with the 7 non overlapping relations of O(M) coming from the 3 basic ones. Adding the 47 compound

relations obtained by disjunction of successive primitive relations gives a total of 62 legitimate relations, to be compared with the 28 relations of O(M).

Example: a Heat Exchanger

We now have a clear, sound and rich system to formally reason about relative orders of magnitude. We are thus going to try to apply it to a simple example of a counter-current heat exchanger as described in [Mavrovouniotis and Stephanopoulos, 1988]. Let FH and KH be the molar-flowrate and the molar-heat of the hot stream, FC and KC the molar-flowrate and the molar-heat of the cold stream. Four temperature differences are defined: DTH is the temperature rise of the cold stream, DTC is the temperature rise of the cold stream, DT1 is the driving force at the left end of the device, and DT2 is the driving force at the right end of the device. The two following equations hold:

(e1) DTH - DT1 - DTC + DT2 = 0,

(e2) $DTH \times KH \times FH = DTC \times KC \times FC$.

The first one is a consequence of the definition of the temperature differences, and the second one is the energy balance of the device. Let us take the following assumptions expressed as order of magnitude relations:

(i) $DT2 \sim DT1$, (ii) $DT1 \ll DTH$, (iii) $KH \approx KC$.

The problem is now to deduce from the 2 equations and these 3 order of magnitude relations the 5 missing order of magnitude relations between quantities having the same dimension (4 for temperature differences and 1 for molar-flowrates). Let us take the axioms (Ai) above and the properties (Pi) of ROM as stated in [Dague, 1993].

Consider first the relation between DT2 and DTH. Thanks to (P4) $A \ll B$, $C \sim A \mapsto C \ll B$, ROM infers from (i) and (ii) that (1) DT2 \ll DTH.

Consider the relation between DTH and DTC. (P5) $A \ll B \mapsto -A \ll B$ and (P6) $A \ll C$, $B \ll C$ $\mapsto (A+B) \ll C$ applied to (ii) and (1) imply -DT1 $+ DT2 \ll DTH$. From this it can be deduced, using (A10), that DTH \approx DTH - DT1 + DT2, i.e. using (e1) that (2) DTH \approx DTC.

Consider the relation between DT1 and DTC. From (ii) and (2) it can be deduced, using (A6) and (A11), that (3) $DT1 \ll DTC$.

Consider the relation between DT2 and DTC. It results from (i) and (3), by using (P4), that (4) DT2 \leq DTC.

Another deduction path can be found to obtain the same result. In fact, from (A10) $A \approx B \mapsto (B-A) \ll$

A and $A \approx C \mapsto (C-A) \ll A$, using (P5) and (P6), (P) $A \approx B$, $A \approx C \mapsto (C-B) \ll A$ can be derived. As, from (3) and (A10), it results that DTC \approx DTC+DT1, it can be deduced from this and (2), using (P), that $-DTH+DT1+DTC \ll DTC$, i.e. using (e1) that (4) DT2 \ll DTC.

Consider finally the relation between FH and FC. (A7), applied to (iii) and (2), gives DTH × KH \approx DTH × KC and DTH × KC \approx DTC × KC. Applying (A3) then gives DTH × KH \approx DTC × KC. Applying (A7) again and using (e2) gives (5) FH \approx FC.

The five results (1 to 5) have thus been obtained by ROM (identical to those produced by O(M) because \neq is not used here):

(1) $DT2 \ll DTH$ (2) $DTH \approx DTC$ (3) $DT1 \ll DTC$ (4) $DT2 \ll DTC$ (5) $FH \approx FC$.

We have now to evaluate them in the real world. For this, it is necessary to fix a numeric scale for the order of magnitude relations. Choose for example \ll represented by at most 10%, \approx by at most (for the relative difference) 10 % and \sim by at most (for the relative difference) 80%. Assumptions thus mean that:

(i') $0.2 \le DT2/DT1 \le 5$, (ii') $DT1/DTH \le 0.1$, (iii') $0.9 \le KH/KC \le 1.112$.

It is not very difficult in this example to compute the correct results by hand. It is found (see also subsections 6.3 and 6.4) that:

(1') $DT2/DTH \le 0.5$ (2') $0.714 \le DTH/DTC \le 1.087$ (3') $DT1/DTC \le 0.109$ (4') $DT2/DTC \le 0.358$ (5') $0.828 \le FH/FC \le 1.556$.

This shows that only the formal result DT1 ≪ DTC is satisfied in practice. For the 4 others, although the inference paths remain short in this example, there is already a non trivial shift, which makes them unacceptable. This is the case for the two \approx relations: DTH may in fact differ from DTC by nearly 30%, and FH may differ from FC by 35%. And the same happens for the two \ll relations: DT2 can reach 35% of DTC and, worse, 50% of DTH. This is not really surprising because we know that there is no model of ROM(K) in \mathbb{R} . Here, it is essentially the rule (P4) that causes discrepancy between qualitative and numeric results. Rules such as (P4), or (A11) from which it comes, and also (A3) are obviously being infringed. What this does demonstrate is the insufficiency of ROM for general engineering tasks and the need for a sound relative order of magnitude calculus in \mathbb{R} .

Transposing the Formal System to \mathbb{R} : ROM(\mathbb{R})

In fact, all the theoretical framework developed in [Dague, 1993] and summed up above is a source of inspiration for this task. Since the rules of ROM capture pertinent qualitative information and may help guide intuition, they will serve as guidelines for inferences in \mathbb{R} ([Dubois and Prade, 1989] addresses the same type of objectives by using fuzzy relations). Let us introduce the natural relations in \mathbb{R} , parameterized by a positive real k, "close to the order k":

 $\begin{array}{rcl} A \stackrel{2}{\leftarrow} B &\longleftrightarrow & |A-B| \geq k \times Max(|A|,|B|), \\ \text{i.e. for } k < 1, & (II) & A/B \leq 1-k & \text{or } A/B \geq 1/1-k & \text{or } \\ B = 0, \text{ and "negligible at the order k":} \\ A \stackrel{k}{\leqslant} B &\longleftrightarrow & |A| \leq k \times |B|, \end{array}$

i.e. (III) $-k \le A/B \le k$ or A=B=0.

The first one will be used to model both \approx and \sim , the second one to model \neq , and the third one to model \ll , by associating a particular order to each relation. When trying to transpose the axioms (Ai) by using these new relations, three cases occur.

Axioms of reflexivity (A1), symmetry (A2,A4), invariance by homothety (A7,A8), and invariance by adding a quantity of the same sign (A12,A13, assuming (A9)) are obviously satisfied by $\stackrel{k}{\sim}$ for any positive k.

A second group of axioms imposes constraints between the respective orders attached to each of the 4 relations. Coupling of ~ with signs (A9) is true for any order k attached to ~ that verifies k < 1. The fact that ~ is coarser than \approx (A6) forces the order for \approx to be not greater than the order for ~. Axiom (A14) is true for $\stackrel{k}{\sim}$ if $k \ge 1/2$. Part of the definition of \ll in terms of \approx , more precisely the left to right implication of (A10) has the exact equivalent: A \ll B \mapsto B $\stackrel{k}{\sim}$ (B+A) for k < 1. We can thus take the same order k_1 for \ll and \approx . In the same way, the definition

of \neq in terms of ~ (A15) has its equivalent: A $\hat{\neq}$ B \leftrightarrow (A-B)^{1-k} A or (B-A)^{1-k} B provided $k \leq$ 1/2, i.e. $1-k \geq 1/2$. If we call k_2 the order for \neq , we can thus take $1-k_2$ as the order for ~. All the above thus leads to the following correspondences: $A \approx B \iff A \stackrel{k_1}{\sim} B \qquad A \sim B \iff A^{1-k_2} B$

 $\begin{array}{rcl} A \approx B & \longleftrightarrow & A \stackrel{k_1}{\sim} B & A \sim B & \longleftrightarrow & A \stackrel{k_2}{\sim} B \\ A \ll B & \longleftrightarrow & A \stackrel{k_1}{\ll} B & A \not\simeq B & \longleftrightarrow & A \stackrel{k_2}{\not\sim} B \\ \text{with } 0 < k_1 \le k_2 \le 1/2 \le 1 - k_2 < 1. \\ \text{Note that, as the formal system ROM(K) depends on two relations, its} \end{array}$

analog in \mathbb{R} has two degrees of freedom represented by the orders k_1 and k_2 .

Remaining axioms are those which are not true in \mathbb{R} . For these, the loss of precision on the orders is computed exactly in conclusion. The rest of the definition of \ll in terms of \approx , i.e. the right to left implication of (A10) gives:

 $B \stackrel{k}{\sim} (B+A) \mapsto A \stackrel{k/1-k}{\leqslant} B (k/(1-k) \le 1 \text{ when } k \le 1/2).$

Transitivity axioms (A3) and (A5) each give:

 $A \stackrel{k}{\sim} B, B \stackrel{k}{\sim} C \mapsto A \stackrel{k+k'-kk'}{\sim} C (k+k'-kk' < 1)$ when k < 1 and k' < 1).

Finally the coupling between \approx (through \ll) and \sim (A11) gives:

 $A \stackrel{k}{\leqslant} B, B^{1} \stackrel{k'}{\sim} C \mapsto A \stackrel{k/k'}{\leqslant} C (k/k' < 1 \text{ when } k < k').$

Like the axioms (Ai), all properties (Pi) deduced in [Dague, 1993] are demonstrated in the same way by computing the best orders in conclusion, when they are not directly satisfied, and constitute all the inference rules of $ROM(\mathbb{R})$. For reasons of lack of space, here are the most significant or useful of the 45 properties for our purpose.

(P4), as (A11), gives $A \stackrel{k}{\leqslant} B$, $A^{1} \stackrel{k}{\sim} C \mapsto C \stackrel{k'k'}{\leqslant} B$. (P6) gives $A \stackrel{k}{\leqslant} C$, $B \stackrel{k'}{\leqslant} C \mapsto (A+B) \stackrel{k+k'}{\leqslant} C$ (which can be improved if [A] = -[B] by taking max(k,k') as order in conclusion) and (P) gives $A \stackrel{k}{\sim} B$, $A \stackrel{k'}{\sim} C$ $\mapsto C-B \stackrel{k}{\leqslant} A$ with $k'' = (k+k'-kk')/(1-\max(k,k'))$ (which can be improved if [C-B] = [A] by taking k'' = (k+k'-kk')/(1-k')).

Transitivity of \ll (P11) obviously improves the degree $A \ll B$, $B \ll C \mapsto A \ll C$.

The incompatibility of \ll and \sim (P14) $A^{1-k_{2}} B$, $A \stackrel{k_{1}}{\ll} B \mapsto A = B = 0$ and of \approx and \neq (P34) $A \stackrel{k_{1}}{\sim} B$, $A \stackrel{k_{2}}{\neq} B \mapsto A = B = 0$ are ensured provided $k_{1} < k_{2}$. These two properties will be used to check the consistency of the set of relations describing, for example, an actual behavior of a physical system, or on the contrary to detect inconsistencies coming, for example, from discrepancies between modeled and actual behaviors of a system for tasks such as diagnosis.

Relations between \approx and \neq (P37, P38) give A $\stackrel{k_2}{\neq}$ B, C $\stackrel{k_1}{\sim}$ A \mapsto C $\stackrel{(k_2-k_1)/(1-k_1)}{\neq}$ B and A $\stackrel{k_1}{\sim}$ B, C $\stackrel{k_2}{\neq}$ A \mapsto (C-A) $\stackrel{k_1/k_2}{\sim}$ (C-B).

Finally, the completeness of the description is obtained: $A^{1-k_2} B$ or $A \not\stackrel{k_2}{\not\leftarrow} B$ provided that $k_2 \leq 1/2$.

Moreover, it can be proved that adding the assumption $A^{1-k_2} \to B$ or $B^{1-k_2} \to A$ or $A \stackrel{k_1}{\ll} B$ or $B \stackrel{k_1}{\ll} A$ would be equivalent to adding A $\stackrel{k_1}{\sim}$ B or A $\stackrel{k_2}{\not\sim}$ B and also equivalent to $k_2 \leq k_1$. This would imply $k_1 = k_2 = e$ as in FOG or in the strict interpretation of O(M) [Mavrovouniotis and Stephanopoulos, 1987], i.e. only one degree of freedom instead or two. In the same way that formal models of ROM(K) could not be reduced to FOG or O(M), the same is obtained for $ROM(\mathbb{R})$ by choosing $k_1 < k_2$, i.e. $0 < k_1 < k_2 \le 1/2$. Note that, in relation to non standard models of ROM(K), one degree of freedom corresponds to what is chosen as the analog in \mathbb{R} of the infinitesimals, and the other to the choice of the analog of the parameter ε [Dague, 1993] of the model, where ε corresponds to k_1/k_2 .



This above gives the exact counterpart in \mathbb{R}_+ of the 15 primitive relations of [Dague, 1993] (in fact inference rules analog to the previous ones can be defined for these relations, often with some better orders in conclusion by taking into account the signs of the quantities, e.g. (P6) and (P) above), for describing the order of magnitude of A/B w.r.t. 1. These relations correspond to real intervals which overlap (in contrast with the strict interpretation of O(M)) and are built from the landmarks k_1 , k_2 , $1-k_2$, $1-k_1$, 1, $1/(1-k_1)$ k_1 , $1/(1-k_2)$, $1/k_2$, $1/k_1$ of \mathbb{R}_+ (see Fig. 1). Note that, as in the formal model, intervals (k_1, k_2) , $(1-k_2, 1-k_1)$ and their inverse are not acceptable relations. The heuristic interpretation of O(M) [Mavrovouniotis and Stephanopoulos, 1987], which only allows the correct inference to be made for one rule, corresponds to the particular case where $k_1 = k_2/(1 + k_2)$. But here k_1 and k₂ are chosen independently, according to the expertise domain.

The orders appearing in each rule of $ROM(\mathbb{R})$ have to be considered as variables, with order in conclusion symbolically expressed in terms of orders in premises. Inference by such a rule is made simply by matching relations patterns in premises with existing relations, i.e. by instantiating the orders to real numbers, and computing the orders in conclusion to deduce a new relation. A sound calculus in R is thus ensured whatever the path of rules used, i.e. any conclusion that can be deduced by application of rules of $ROM(\mathbb{R})$ from given correct premises is correct when interpreted in R. This may be entirely hidden from the user, with both data and results being translated via k1 and k2 in symbolic order of magnitude relations as in FOG, but this time correctly. But the user may also incorporate numeric information as required by using k orders directly or even introducing numeric values for quantities. In this last case, binary relations between two given numeric quantities are automatically inferred from the equivalent formulation of these relations in terms of intervals (I,II,III).

Control of the inference in order to avoid combinatory explosion remains a problem for large applications. A pragmatic solution is to call on the expert who will possibly prevent a rule from being applied if he considers in the light of its underlying qualitative meaning that the conclusions are not relevant.

The Example Revisited

Let us take the example of the heat exchanger again and follow the same reasoning paths, but this time using the inference rules of $ROM(\mathbb{R})$. Take, as in the numeric application, $k_1 = 0.1$ and $k_2 = 0.2$. As (1) is inferred by using (P4) we obtain:

(1a) $DT2 \ll DTH$ with $k_3 = k_1/k_2 = 0.5$.

DT2 and -DT1 having opposite signs, application of (P6) gives $-DT1 + DT2 \ll DTH$

with $k4 = max(k_1,k_3) = 0.5$. Using left to right implication of (A10) and (e1), we get:

(2a) DTH $\stackrel{k_4}{\sim}$ DTC with k4 = max(k₁,k3) = 0.5.

From (ii) and (2a), it can be deduced, using (A11), that:

(3a) DT1 $\stackrel{ks}{\leq}$ DTC with $k5 = k_1/(1-k4) = 0.2$.

The first deduction path leading to (4) has as an equivalent, using (P4), DT2 \leq DTC with $k6=k5/k_2=1$, which cannot be used because the order of \leq is assumed to be < 1. We may, however, use the other deduction path. As, from (3a) and (A10), we have DTC $\stackrel{15}{\sim}$ DTC + DT1, it can be deduced from this and (2a), using (P) and (e1), that: (4a) DT2 \leq DTC

with k7 = (k4 + k5 - k4k5)/(1 - k5) = 0.75.

Note that two different paths leading to the same formal result in ROM may lead here to different results in $ROM(\mathbb{R})$. This poses the as yet unsolved problem of defining heuristics in order to obtain the best result, by pruning the paths that lead to less precise ones (the length of the deduction path not necessarily being a good criterion).

From DTH×KH ^{k1} DTH×KC and DTH×KC ^{k4} DTC×KC, (A3) gives DTH×KH ^{k8} DTC×KC, from which, using (A7) and (e2), we obtain:

(5a) FH $\stackrel{k_8}{\sim}$ FC with $k_8 = k_1 + k_4 - k_1 k_4 = 0.55$.

Results (1a to 5a) have thus been obtained by applying rules of $ROM(\mathbb{R})$. In terms of intervals, these relations are expressed as:

They can automatically be translated in terms of formal order of magnitude compound relations w.r.t. scales k_1 and k_2 (with obviously a loss of precision in general), giving:

DT2 \ll .. \prec DTH DTH \preccurlyeq .. \succcurlyeq DTC DT1 \prec DTC DT2 \ll .. \prec DTC FH \preccurlyeq .. \succcurlyeq FC.

In contrast with results of FOG or O(M) (1 to 5), this time the results are correct. We thus have a sound calculus in \mathbb{R} , with all the advantages of the qualitative meaning transmitted by rules of ROM. In particular, each of the above results has its explanation in commonsense reasoning terms given by the rules applied to obtain it. Using symbolic computation, the formal k orders of the results can even be expressed in terms of k_1 and k_2 . This can be used for other purposes such as design, so as to tune the values of k_1 and k_2 and thus make sure desired orders of magnitude relations are satisfied.

Nevertheless it can be noticed, by comparing them with exact results (1'to 5'), that these relations are not in general optimal. In fact, in qualitative terms, the exact results would give:

improving 3 of the 5 above results. The improvement is even more obvious when comparing ranges given by numeric orders k3 to k8 with exact results. Only DT2/DTH is correctly estimated (i.e. (1a) and (1') are the same). In fact, this is not surprising. Although each rule of ROM(\mathbb{R}) has been computed with the best estimate for order in conclusion, so that each rule taken separately cannot be improved, this does not guarantee optimality through an inference path using several rules that share common variables. In some way, what we have is local optimality, not global optimality. If we estimate that the obtained results, although sound, are not accurate enough for our purpose, we have to supplement ROM(\mathbb{R}) with other techniques.

Using Numeric or Symbolic Algebra Techniques

Once sound results of $ROM(\mathbb{R})$, with the obvious qualitative meaning of the inference paths, have been obtained, several supplementary techniques can be used in order to refine them if needed. These techniques come from two different approaches: numeric ones which transpose well-known consistency techniques for CSPs to numeric CSPs, and symbolic ones which use computer algebra. These approaches are not exclusive and can be usefully combined.

Applying Consistency Techniques for Numeric CSPs

A first way of refining the results is to start from definitions (I,II,III) of the fundamental relations of $ROM(\mathbb{R})$ in terms of intervals, a technique that can easily be extended to all 15 primitive relations. Numeric values are also naturally represented by intervals to take into account precision of observation. Interval computation thus offers itself. Moreover, we are not limited to intervals representing the 15 primitive relations or the compound ones, i.e. to the scale of $ROM(\mathbb{R})$; we can in fact express any order of magnitude binary relation between two quantities by an interval encompassing the quotient of the quantities. In particular, intervals do not need the specific symmetry properties of those of $ROM(\mathbb{R})$ such as in (I,II,III). Since using intervals is thus more accurate when expressing data, it should also be so for the results. But, unfortunately, interval propagation is rarely powerful enough: in the heat exchanger example nothing is obtained by this method.

The idea is to generalize interval propagation in the same way that, in CSPs, k-consistency with k > 2extends arc consistency. This has been done in [Lhomme, 1993], who shows that the consistency techniques that have been developed for CSPs can be adapted to numeric CSPs involving, in particular, continuous domains. The way is to handle domains only by their bounds and to define an analog of k-consistency restricted to the bounds of the domains, called k-B-consistency. In particular 2-B-consistency, or arc B-consistency, which formalizes interval propagation, is extended by the notion of k-B-consistency. The related algorithms with their complexity are given for k = 2 and 3. They have been implemented in Interlog [Dassault Electronique, 1991], above Prolog language. In this section, these techniques are evaluated w.r.t. the heat exchanger example.

Starting from equations (e1) and (e2) and assumptions (i',ii',iii'), bounds for the 5 remaining quotients are looked for. In this case, as already seen, arc B-consistency gives no result. But 3-B-consistency gives the following results for the first 4 quotients (nothing is obtained for FH/FC) with parameters characterizing the authorized relative imprecision at the bounds w1 = 0.02 and w2 = 0.0001 (in about 75s on an IBM 3090):

- (1") $DT2/DTH \le 0.508$
- (2'') 0.665 \leq DTH/DTC \leq 1.120
- (3'') DT1/DTC ≤ 0.112
- (4") $DT2/DTC \le 0.559$.

It can be noticed that estimates (2'',3'',4'') are better than corresponding results of ROM(\mathbb{R}) (2a,3a,4a) and, for the first two, not far from optimal ones (2',3'). 4-B-consistency has also been tried, although execution time increases considerably. For example, $0.710 \leq \text{DTH/DTC} \leq 1.090$ and $\text{DT2/DTC} \leq 0.362$, which well approximate (2') and (4'), are obtained in a few minutes with w1 = 0.01 and w2 = 0.05.

Although interval propagation alone is in general insufficient, k-B-consistency techniques with $k \ge 3$ may thus provide very good results, but some difficulties remain (here, nothing can be done with equation (e2), unless considering at least 5-consistency with efficiency problems).

Using Symbolic Algebra first

The above results reach the limits of purely numeric approaches. If we want to progress towards optimal results, we have to use computer algebra in order to push symbolic computation as far as possible and delay numeric evaluation In a great number of real examples, the total number of equations expressing the behavior of the system and of order of magnitude assumptions equals the number of order of magnitude relations asked for, and the desired dimensionless quotients can be solved in terms of the known quotients, using these equations. These solutions are very often expressed as rational functions and this symbolic computation can be achieved by computer algebra.

For example, from equations (e1) and (e2), known relations

 $DT2 = Q1 \times DT1$, $DT1 = Q2 \times DTH$, $KH = Q3 \times KC$, and searched relations

 $DT2=X \times DTH$, $DTH=Y \times DTC$, $DT1=W \times DTC$, $DT2=Z \times DTC$, $FH=U \times FC$,

MAPLE V [Char, 1988] immediately deduces the formulas (F):

 $X = Q1 \times Q2$, $Y = 1/(1 - Q2 + Q1 \times Q2)$,

 $W = Q2/(1-Q2+Q1\times Q2),$

 $Z = Q1 \times Q2/(1 - Q2 + Q1 \times Q2),$

 $U = (1 - Q2 + Q1 \times Q2)/Q3,$

with $1/5 \le Q1 \le 5$, $0 \le Q2 \le 1/10$, $9/10 \le Q3 \le 10/9$.

Numeric CSP techniques can now be applied directly to these symbolic equations. This time, results are obtained just with arc B-consistency, even for U:

(1s) $X \le 0.5$ (2s) $0.666 \le Y \le 1.112$ (3s) $W \le 0.112$ (4s) $Z \le 0.556$ (5s) $0.810 \le U \le 1.667$.

It can thus be seen that, when starting from solved symbolic expressions, the most simple numeric technique, i.e. analog to interval propagation, gives results which are close to the exact ones (1'to 5') and, in all cases, much better than those given by $ROM(\mathbb{R})$ (1a to 5a). Obviously, using 3-B-consistency improves the results still further, in particular for Z, as follows (with w1=0.001 in 10s):

which are practically optimal.

Using Symbolic Algebra Alone for Computing Optimal Results

Symbolically expressing searched quotients in terms of known ones (Qi) leads to expressions which are continuously differentiable in Qi and most often algebraic (rational functions such as in (F)). The problem to be solved can thus generally be expressed as that of finding the absolute extrema of these expressions on n-dimensional closed convex parallelepipeds defined by the ranges of the known intervals mi \leq Qi \leq Mi for $1 \leq i \leq n$. It is well-known that these extrema occur at points where partial derivatives are null. Thus this is a way to compute them exactly from roots of derivatives by using computer algebra.

More precisely, a necessary (not sufficient because it can correspond in particular to a local extremum) condition for an absolute extremum in a neighborhood is the nullity of all the partial derivatives at the given point. A difficulty arises because extrema may be obtained on a face of dimension < n rather than in the interior of the parallelepiped. Thus derivatives on all faces have to be considered. But, thanks to computer algebra, it is sufficient to symbolically compute partial derivatives once and for all and then, in order to obtain derivatives on any face, to fix the Qi, which determine the face, to their numeric values. Roots of all derivatives (in our case roots of a system of polynomials) are computed, firstly in the interior and then on the different faces in decreasing order of dimension, and the corresponding numeric values of expressions at these points are evaluated up to the vertices. These values are finally compared and only the highest and lowest are kept, which correspond to the absolute extrema.

Let us now apply this method, implemented in MAPLE V, to the heat exchanger example. Expressions X, Y, W and Z depend on the 2 variables Q1 and Q2 and are thus considered w.r.t. the rectangle $1/5 \le Q1 \le 5$, $0 \le Q2 \le 1/10$; U, which depends on the 3 variables Q1, Q2 and Q3 is considered w.r.t. the parallelepiped based on the previous rectangle with $9/10 \le Q3 \le 10/9$. Results are computed immediately and summarized below.

For X, Y, W and Z, it is found that only their derivatives w.r.t. Q1 are null on the edge Q2=0. Corresponding constant values X=0, Y=1, W=0and Z=0 are shown, after inspection of vertices, to be the minima for X, W and Z, but not an absolute extremum for Y. Looking now at the vertices, it is found that the maximum of X is obtained at the vertex Q1=5, Q2=1/10 and is equal to 1/2; the minimum of Y is reached at Q1=5, Q2=1/10 and is equal to 5/7, and its maximum is reached at Q1=1/5, Q2=1/10 and is equal to 25/23; the maximum of W is obtained at Q1=1/5, Q2=1/10 and is equal to 5/46 and the maximum of Z is obtained at Q1=5, Q2=1/10 and is equal to 5/14.

The derivative of U w.r.t. Q1 is null both on the edge Q2=0, Q3= 9/10 corresponding to the constant value U=10/9 and on the edge Q2=0, Q3=10/9 corresponding to the constant value U=9/10. But it is finally found that the minimum occurs at the vertex Q1=1/5, Q2=1/10, Q3=10/9 and is equal to 207/250, and that the maximum occurs at the vertex Q1=5, Q2=1/10, Q3=9/10 and is equal to 14/9.

Finally computer algebra, which works with rational numbers, gives the exact solutions (S) to our problem:

Floating point approximation with 3 significant digits gives (1' to 5').

The method of roots of derivatives, processed by computer algebra, is thus a very powerful technique to automatically obtain the exact ranges. But, in addition to the complete loss of the qualitative aspect of the inference and the necessity, as in the above subsection, for the system of equations to be algebraically solvable, there are two other drawbacks to this approach. The first one is that roots of a polynomial system cannot in general be obtained exactly. This is solved in practice in a large number of cases by using the most recent modules of computer algebra which are able to deal with algebraic numbers (represented as a couple of a floating point interval and a polynomial, coefficients of which are algebraic numbers, such that the considered number is the only root of the polynomial belonging to the interval). The second one is the exponential complexity of the method: in an n-dimensional space we have 3ⁿ systems of polynomials to look for, from the interior to the vertices. The method becomes intractable very rapidly unless the number of variables (assumed order of magnitude relations) remains very small.

Syntactically Transforming Rational Functions: a Line of Research

There are cases where, after having judiciously syntactically transformed rational functions which are solutions of the set of equations, the simple interval propagation technique gives the exact optima, as illustrated in the example.

Let us consider symbolic formulas (F). The exact result (1s) can be obtained simply by interval propagation for X because variables Q1 and Q2 have only one occurrence in X. It is not the case for the other 4

formulas, which is why, in this case, interval propagation does not give exact results (2s to 5s). However, a simple trick may be found by hand to satisfy this condition. In fact the expression $1-Q2+Q1\times Q2$ in Y, W and U may be rewritten as $1+Q2\times(Q1-1)$, which boils down to changing a variable: Q1-1 instead of Q1. A simple interval propagation gives $23/25 \le 1 + Q2 \times (Q1-1) \le 7/5$, from which exact solutions (S) for Y, W and U are immediately obtained. It is not the case for Z because Q1 appears also in the numerator. But Z can be rewritten as Z = 1/(1 + (1/Q1)(1/(Q2-1))) where each new variable 1/Q1 and 1/(Q2-1) appears only once. The exact result (S) $0 \le Z \le 5/14$ follows immediately. This interval propagation may be achieved exactly by manipulating rational numbers, or with a given approximation by manipulating floating point numbers, as is done by Interlog with 10 exact significant digits.

It can be concluded that, when expressions can be rewritten by changing variables, such that each new variable occurs only once, simple interval propagation gives exact solutions. This transformation is obviously not always possible. A line of research would be to characterize the cases where such a transformation of rational functions (or at least a partial one which minimizes the number of occurences of each variable) is possible and to find algorithms to do this.

Conclusion

It has been shown in this paper that the formal system ROM(K) [Dague, 1993] can be transposed in \mathbb{R} in order to incorporate quantitative information easily, and to ensure validity of inferences in \mathbb{R} . Rules of ROM(\mathbb{R}) thus guarantee a sound calculus in \mathbb{R} (which was not the case with FOG, O(M) or ROM(K)), while keeping their qualitative meaning, thus guiding research and providing commonsense explanations for results.

If the loss of precision through inference paths is such that some of these results are judged to be too imprecise for a specific purpose, several complementary techniques can be used to refine them. k-consistency algorithms for numeric CSPs, which generalize for k > 2 interval propagation, generally improve the results but may require a large k, in which case they are very time consuming. A better approach is first to use computer algebra to express dimensionless quotients for which approximation is searched in terms of quotients for which given bounds are assumed, and then to apply k-consistency techniques to the symbolic expressions obtained. It has also been shown that computer algebra alone may be used to obtain exact results, by computing roots of partial derivatives in order to obtain the extrema of the expressions on n-dimensional parallelepipeds although this method, which is exponential in n, is tractable only for a small number of variables (i.e. known quotients). Finally, future work would consist in formally modifying rational functions in order to have a minimal number of occurrences of each variable, thus making interval computation more precise; in particular, when it is possible to have only one occurrence for each variable, simple interval computation gives the exact results.

All this assortment of tools, with $ROM(\mathbb{R})$ as the basis, is now available to perform powerful and flexible qualitative and numeric reasoning for engineering tasks, and will be tested soon on real applications in chemical processes.

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References

- D. Bobrow, Qualitative Reasoning about Physical Systems, MIT Press, Cambridge, 1985.
- B.W. Char, MAPLE Reference Manual, Watcom, Waterloo, Ontario, 1988.
- P. Dague, "Symbolic reasoning with relative orders of magnitude," *Proceedings of the Thirteenth IJCAI*, Chambéry, August 1993.
- P. Dague, P. Devès, and O. Raiman, "Troubleshooting: when Modeling is the Trouble," *Proceedings of AAAI Conference*, Seattle, July 1987.

- Dassault Electronique, INTERLOG 1.0, User's Guide, 1991.
- J. de Kleer and J.S. Brown, "A qualitative physics based on confluences," Artificial Intelligence 24, 1984.
- J.-L. Dormoy and O. Raiman, "Assembling a device," *Proceedings of AAAI Conference*, St. Paul, August 1988.
- D. Dubois and H. Prade, "Order of magnitude reasoning with fuzzy relations," Proceedings of the IFAC/IMACS/IFORS International Symposium on Advanced Information Processing in Automatic Control, Nancy, 1989.
- K.D. Forbus, "Qualitative process theory," Artificial Intelligence 24, 1984.
- B.J. Kuipers, "Qualitative simulation," Artificial Intelligence 29, 1986.
- O. Lhomme, "Consistency techniques for numeric CSPs," Proceedings of the Thirteenth IJCAI, Chambéry, August 1993.
- M.L. Mavrovouniotis and G. Stephanopoulos, "Reasoning with orders of magnitude and approximate relations," *Proceedings of AAAI Conference*, Seattle, July 1987.
- M.L. Mavrovouniotis and G. Stephanopoulos, "Formal order of magnitude reasoning in process engineering," *Comput. chem. Engng.* 12, 1988.
- S.S. Murthy, "Qualitative reasoning at multiple resolution," *Proceedings of AAAI Conference*, St. Paul, August 1988.
- O. Raiman, "Order of magnitude reasoning," *Proceedings of AAAI Conference*, Philadelphia, August 1986.
- O. Raiman, "Order of magnitude reasoning," Artificial Intelligence 51, 1991.
- P. Struss, "Mathematical aspects of qualitative reasoning," AI in Engineering 3-3, 1988.
- L. Travé-Massuyès and N. Piera, "The orders of magnitude models as qualitative algebras," *Proceedings of the Eleventh IJCAI*, Detroit, August 1989.
- B.C. Williams, "MINIMA: a symbolic approach to qualitative algebraic reasoning," *Proceedings* of AAAI Conference, St. Paul, August 1988.